4-Cyclohexylphenylacetic acid 35889-00-0 | DTXSID60189446

Model Performance

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Weighted KNN model

5-fold CV (7	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.72	51.8	0.74	50.3	0.73	52.7	

Model Results

Predicted value: 132 °C

Global applicability domain: Inside

Local applicability domain index: 7.07e-01

Confidence level: 6.55e-01

Nearest Neighbors from the Training Set

Image not found

5,6,7,8-Tetrahydro-2-naphthoic

acid

Measured: 156 Predicted: 139

Image not found

1-Naphthalenecarboxylic acid,

3,4-dihydro-Measured: 125 Predicted: 129

Image not found

1-Naphthaleneacetic acid

Measured: 135 Predicted: 160

Image not found

2-Naphthylacetic acid

Measured: 142 Predicted: 162